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6. AUTHOR(S)
  Dr. H.T. Banks
  Dr. K.J. Bachmann		

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES Center for Research in Scientific Computation Box 8205 North Carolina State University Raleigh, NC 27695-8205		8. PERFORMING ORGANIZATION REPORT NUMBER
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13. ABSTRACT (Maximum 200 words)

P-polarized reflectance spectroscopy (PRS) was developed as a method of real-time process monitoring. The relation between the measured reflectance and the chemical kinetics driving the growth of an epitaxial film on the surface of a substrate has been established for the conditions of pulsed chemical beam epitaxy. The precision of the monitoring of molecular layer growth by PRS has been evaluated. Also, limitations to the accuracy of PRS monitoring have been assessed. The design of the RTOMCVD reactor has been completed. Experimental validation of predictions of temperature distributions and flow have been initiated. We have applied the reduced basis method for control of the viscous incompressible gas flow dynamics by boundary surface controls which suggests that real-time simulation and control can be done by lower-order reduced order control systems.

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RAPID THERMAL PROCESSING OF SEMICONDUCTORS
AT HIGH VAPOR DENSITIES

Final Report

June 15, 1995 -December 31, 1996

Principal Investigator:

Dr. H. T. Banks

Center for Research in Scientific Computation

Box 8205

North Carolina State University

Raleigh, NC 27695-8205

email: htbanks@eos.ncsu.edu

FAX (919) 515-1636

Phone: (919) 515-3968

Statement of Problem

The overall scientific and technical effort of our research entails research in scientific computations concerning the control of the flow dynamics of key semiconductor manufacturing processes that operate at higher flukes of nutrient molecules sustaining film growth than accessible with conventional processing tools. These are rapid thermal organometallic chemical vapor deposition (RTOMCVD) and pulsed Chemical beam epitaxy (PCBE). The modeling is closely coordinated with hardware design and process engineering tasks including the testing of novel non-invasive methods of real-time process monitoring and control, e.g., p-polarized reflectance spectroscopy. The development of mathematical models has been initiated that accurately describe gas flow and deposition process for RTOMCVD reactors in various operating conditions and that link p-polarized reflectance signal to the composition of the suface. These models include the full compressible gasdynamic equations which incorporate multiple species and reactions between the species coupled with boundary conditions that describe conditions at the inlet, outlet and the deposition process. Refinement of these models and the implementation of closed-loop process control are objectives of continuing research funded by a DoD MURI on Intelligent materials processing and electronics.

Summary

I. Research Accomplishments

P-polarized reflectance spectroscopy (PRS) was developed as a method of real-time process monitoring[1]-[6]. The relation between the measured reflectance and the chemical kinetics driving the growth of an epitaxial film on the surface of a substrate has been established for the conditions of pulsed chemical beam epitaxy[3]-[5]. The precision of the monitoring of molecular layer growth by PRS has been evaluated[6]. Also, limitations to the accuracy of PRS monitoring have been assessed. The design of the RTOMCVD reactor has been completed. Experimental validation of predictions of temperature distributions and flow have been initiated. We have applied the reduced basis method for control of the viscous incompressible gas flow dynamics by boundary surface controls which suggests that real-time simulation and control can be done by lower-order reduced order control systems.

II. Research Accomplishments and Findings

The design of the RTOMCVD reactor has been completed and numerical simulations of temperature distributions and flow in this reactor have been performed. We have chosen a

design of the RTOMCVD reactor that employs a channel flow across the substrate wafer - attached to a rotating susceptor that is heated by radio-frequency heating. The reactor is comprised of (i) an inner fused silica construction that shapes the flow and provides for a clean, non-reactive enclosure for chemical vapor deposition process and (ii) an outer steel shell that provides for containment of a nitrogen atmosphere. This outer steel shell is held at the chosen pressure with controlled pressure equalization between the inside of the inner fused silica and the outer steel shells. The latter is presently under construction. The flow control part of the design is laid out for four process gases and five organometallic (OM) source vapors. Provisions are made for pulsed injection of the process gases and OM source vapors. This is essential for the operation at elevated pressure because of the inverse relation between the diffusion constant and pressure, requiring OM source saturation at low pressure combined with pulsed injection into the silica flow channel by plugs of high pressure carrier gas. Pulsed operation provides also for instantaneous probing of the reaction kinetics that drives the heteroepitaxial process *via* optical real-time process monitoring and mass spectrometric sampling of source vapor and waste vapor compositions. The switching of gases is designed to minimize pressure oscillations in the reactor. Applications of RTOMCVD will focus onto heterostructures employing wide bandgap group III phosphides, nitrides and phosphonitrides in the context of optoelectronic devices[7]. We are assessing at present by infrared imaging the temperature distribution for a specific prototype fused silica shell of rectangular cross section of the channel for atmospheric pressure flow. An extension of this assessments to a scalable multiwafer reactor is planned.

Initial numerical flow simulations on such a RTOMCVD chamber have been performed in order to investigate the effects of reactor geometry and operating conditions on flow patters and growth rate uniformity. For thermally activated process, high growth rates require operation at high mass flow rate. Because this reason we use the compressible gas dynamics equations to model the flow inside a 2-D axi-symmetric reactor chamber approximating the set of wafers by a doughnut shaped ring. We carried out our numerical computations using a commercial software package FIDAP, for the finite element simulations and an in-house numerical code based on a mixed finite element method. Our numerical simulations shows that under the current design of the horizontal reactor with expanding cross section and the vertical injection of the inlet gas which makes the ninety-degree bend, a recirculation region exists near the susceptor. We are currently studying the effect of the operating conditions, the shape of the inlet region and thermal distributions on reducing this recirculation cell. These and other simulation results provided valuable information to the design of an optimal reactor chamber.

Control problems that involve a real-time regulation of flow and growth uniformity in the RTOMCVD are formidable problems to solve. The state equations are the Navier-Stokes equations, the geometry is often complex and the time interval involved is often very large. If one were to solve such problems using standard finite element or finite difference method the resulting system is prohibitively large. We have investigated a reduction type method based on the so-called reduced basis method, which over comes this difficulty. The reduced basis method uses basis functions which are closely related to the problem that is being solved. This is in contrast to the traditional numerical methods such as finite difference method which uses grid functions as basis functions or finite elements method which uses piecewise polynomials for this purpose. There are several approaches available for the selection of basis functions. We tested the Lagrange approach that uses solutions of the problem at various parameter values as basis functions. The major advantage of this method over others such as finite element, finite difference or spectral method is that it has

fewer degrees of basis functions. The reduced basis which we developed has been tested successfully on two optimal control problems in steady viscous incompressible flow with boundary control. The first one is a velocity tracking problem in cavity flow and the second one is vorticity control problems in channel flow. Currently we are conducting our research on developing reduced-order robust feedback methodologies for thermally convected flows in channels and RTOMCVD reactor.

We have conducted the mathematical studies for the PRS real-time monitoring technique. We analyzed the PRS signal for PCBE epitaxial film growth process of GaP/Si hetero-structures. We have carried out the sensitivity analysis of the PRS signal with respect to the modulation of the substrate temperature, incident angle of the laser beam and dielectric constants of the film and substrate layers, and measurement noise. The relation between the measured reflectance and the activities of the reactants and products of chemical reactions that feed the heteroepitaxial growth process has been established for a linearized approximation of the complex reflectivity. Off-line estimations of parameters; the incident angle of the laser beam, complex dielectric constants of the film and substrate and growth rate per pulsing cycle were carried out successfully using the least square method for data-fitting problem, under homogeneous growth conditions. We are currently developing on-line recursive algorithms for estimating the growth rate and film dielectric constants and feedback control laws for regulation of the uniform film growth.

Participating Scientifc Personnel

K.J. Bachmann, G. Lucovsky, H.T. Banks, K. Ito, G.M. Kepler, H.T. Tran, J.S. Scroggs, S. Ravindran, C. Hoepfner, and N. Sukidi

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Interactions and Transitions

Lectures

1. N. Dietz and K.J. Bachmann, Real-time optical monitoring of epitaxial growth processes by p-polarized reflectance spectroscopy, Mat. Res. Soc. Fall Meeting, Boston, MA, 1995

2. N. Dietz, U. Rossow, D.E. Aspnes, N. Sukidi and K.J. Bachmann, Real-time optical monitoring of $Ga_xIn_{1-x}P/GaP$ heterostructures on silicon, Mat Res. Soc. Fall Meeting, Boston, MA, 1995

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4. U. Rossow, N. Dietz, K.J. Bachmann and D.E. Aspnes, Optical investigation of surface processes in GaP heteroepitaxy on silicon under pulsed chemical beam epitaxy conditions, PCSI Meeting, LaJolla, CA, 1996

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Patents

None

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